The Electron-Screening Correction for the Proton-Proton Reaction

John N. Bahcall[*]

School of Natural Sciences, Institute for Advanced Study, Princeton, NJ 08540

Xuelei Chen[†] and Marc Kamionkowski[‡]

Department of Physics, Columbia University, 538 West 120th Street, New York, NY 10027

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Abstract

We test the Salpeter formalism for calculating electron screening of nuclear fusion reactions by solving numerically the relevant Schrodinger equation for the fundamental proton-proton reaction. We evaluate exactly the square of the overlap integral of the two-proton wave function and the deuteron wave function and compare with the usual analytic approximation. The usual WKB solution agrees with the numerical solution to $O(10^{-4})$.

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[*]jnb@ias.edu

[†]xuelei@phys.columbia.edu

[‡]kamion@phys.columbia.edu

I. INTRODUCTION

Over the past three decades, much work has been devoted to refining the input data used in calculating solar-neutrino fluxes. The comparison between the predicted and the observed fluxes has important implications for particle physics and astrophysics. Most recently, a great deal of attention has been paid to a relatively minor effect, the electron screening of nuclear fusion reactions [1–6], and it has even been argued [7] that the discrepancy between observations and theoretical predictions might be reduced significantly if a different screening correction is adopted.

We test in this paper the robustness of the standard WKB analytic treatment due to Salpeter [1] by solving numerically the relevant Schrodinger equation, including a Debye-Huckel screening potential, for the fundamental proton-proton (pp) reaction. The unscreened rate of this reaction can be calculated precisely [8] using standard weak-interaction theory, accurate laboratory data for the two-proton system, and different refined deuteron wave functions in agreement with a variety of nuclear-physics measurements. Radiative corrections are also included in the standard calculation [8].

In the next Section, we re-derive Salpeter's analytic result for the weak-screening limit using a kinetic-theory approach (rather than Salpeter's thermodynamic arguments). In Section III, we calculate the proton-proton wave function in both a screened and unscreened Coulomb potential by numerical solution of the Schrodinger equation. We then use these results to evaluate numerically the electron-screening correction to the proton-proton reaction, thereby testing the validity of the standard WKB calculation. In an Appendix, we calculate a correction to Salpeter's result and find it to be negligibly small.

II. REVIEW OF SCREENING CORRECTION

To begin, we re-derive Salpeter's screening correction. To do so, we use kinetic theory to calculate reaction rates in both a screened and unscreened plasma. Although Salpeter's derivation was based on a thermodynamic argument, this alternative approach recovers the same results, and it will be useful for understanding the numerical work in the following Section. With our analytic approach, a very small correction to Salpeter's results is obtained and presented in the Appendix.

The nuclear fusion rates in the solar interior are controlled primarily by Coulomb barriers. Therefore, the energy dependence of the fusion cross section is usually written as

$$\sigma(E) \equiv \frac{S(E)}{E} \exp(-2\pi\eta), \tag{1}$$

where $S(E)$ is a function that varies smoothly in the absence of resonances, and

$$\eta = \frac{Z_1 Z_2 e^2}{\hbar v}. \tag{2}$$

Here, $Z_1 e$ and $Z_2 e$ are the charges of the two colliding nuclei, and v is their relative velocity.

The controlling factor, $\exp(-2\pi\eta)$, in Eq. (1) takes into account the probability for the nuclei to tunnel through the Coulomb barrier. It is obtained from the Coulomb potential $V(r) = Z_1 Z_2 e^2/r$ through the WKB approximation,

$$\Gamma(E) = \exp\left(\frac{-2}{\hbar} \int_0^{r_c} [2\mu(V_{\text{Coul}}(r) - E)]^{1/2} dr\right)$$

$$= \exp\left(-2Z_1 Z_2 \frac{e^2}{\hbar} \sqrt{\frac{2\mu}{E}} \int_0^1 \sqrt{\frac{1}{u} - 1} \; du\right) \tag{3}$$

$$= e^{-2\pi\eta}, \tag{4}$$

where r_c is the classical turning point, defined by $V_{\text{Coul}}(r_c) = E$, E is the kinetic energy, and μ is the reduced mass,

$$\mu = \frac{m_1 m_2}{m_1 + m_2}. \tag{5}$$

Here, m_1 and m_2 are the masses of the reacting nuclei.

If the energies of the reacting nuclei have a Maxwell-Boltzmann distribution at a temperature T, the thermally-averaged cross section times relative velocity is [9]

$$\langle \sigma v \rangle = \sqrt{\frac{8}{\pi\mu(k_B T)^3}} \int_0^\infty dE \; S(E) \exp(-2\pi\eta - E/k_B T). \tag{6}$$

However, in the stellar interior each nucleus, even though completely ionized, attracts neighboring electrons and repels neighboring nuclei; thus, the potential between two colliding nuclei is no longer a pure Coulomb potential, but a screened potential $V_{\text{sc}}(r)$. In the weak-screening case, the Coulomb interaction energy between a nucleus and its nearest few electrons and nuclei of the gas is small compared with the thermal energy $k_B T$. In this case, the surrounding electrons and ions are only slightly displaced, and we obtain a screened potential of the form [1]

$$V_{\text{sc}}(r) = \frac{Z_1 Z_2 e^2}{r} \exp(-r/r_D). \tag{7}$$

Here,

$$r_D = \zeta^{-1/2} \left(\frac{k_B T a}{e^2}\right)^{1/2} a, \tag{8}$$

is the Debye radius for the cloud; $A = A_1 A_2/(A_1 + A_2)$ is the reduced mass in atomic mass units; $\zeta = \sqrt{\sum_i (X_i Z_i^2/A_i + X_i Z_i/A_i)}$; X_i, Z_i, and A_i are the mass fraction, charge, and mass number, respectively, of nucleus i;

$$a = \frac{1}{(4\pi\rho N_0)^{1/3}} = \rho^{-1/3}(0.51 \times 10^{-8} \text{ cm}) \tag{9}$$

is a measure of interparticle distance; ρ is the density in units of g cm^{-3}; and N_0 is Avogadro's constant.

For the screened potential, the penetration factor is then given by

$$\Gamma(E) = \exp\left(\frac{-2r_c}{\hbar} \sqrt{2\mu E} \int_0^1 \left[\frac{1}{u}\exp\left(x(1-u)\right) - 1\right]^{1/2} du\right), \tag{10}$$

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where $x = x(E) = r_c/r_D$. Here, r_c is the classical turning-point radius defined by $V_{sc}(r_c) = E$. However, if x is small, then r_c for the screened potential is roughly that for the unscreened potential: $r_c \simeq Z_1 Z_2 e^2/E$. By expanding the exponential in the small-x limit (to be justified below), we obtain

$$\Gamma(E) = \exp[-2\pi\eta(1 - x/2)] = e^{-2\pi\eta} e^{x\pi\eta}. \tag{11}$$

Although $x\pi\eta$ depends on the energy, the effect of the correction on the thermally-averaged cross section can be approximated by evaluating $x\pi\eta$ at the most probable energy of interaction,

$$E_0 = [(\pi\alpha Z_1 Z_2 k_B T)^2 (mAc^2/2)]^{1/3} \tag{12}$$

$$= 1.2204 (Z_1^2 Z_2^2 A T_6^2)^{1/3} \ \text{keV} \tag{13}$$

where m is the atomic mass unit, and T_6 is the temperature in units of 10^6 K. Then,

$$\langle\sigma v\rangle \simeq \sqrt{\frac{8}{\pi\mu(k_B T)^3}} f_0 \int_0^\infty dE S(E) \exp(-2\pi\eta - E/k_B T), \tag{14}$$

where the Salpeter factor f_0 is given by

$$f_0 = e^{x_0 \pi\eta} = \exp(0.188 Z_1 Z_2 \zeta \rho^{1/2} T_6^{-3/2}), \tag{15}$$

where ρ is the density in units of g cm^{-3}, and

$$x_0 = x(E_0) = 0.0133 \, (Z_1 Z_2)^{1/3} A^{-1/3} \rho^{1/2} T_6^{-7/6} \zeta. \tag{16}$$

For the pp reaction, $x_0 \simeq 0.01$, which justifies the small-x approximation used above. Equations (6)–(16) provide an alternative derivation of the Salpeter [1] weak-screening formula.

III. NUMERICAL RESULTS

We now calculate numerically the cross section for the pp reaction for a Coulomb potential and a screened Coulomb potential to compare with the WKB calculation of the screening correction. To do so, we note that the reaction rate is proportional to Λ^2 [10], where Λ is the overlap integral of the proton-proton wave function and the deuteron wave function,

$$\Lambda = \sqrt{\frac{a_p^2 \gamma^3}{2}} \int u_d(r) u_{pp}(r) dr, \tag{17}$$

where a_p is pp scattering length, $\gamma = \sqrt{2\mu E_d}$ is the deuteron binding wave number, and E_d is the deuteron binding energy. The function $u_d(r)$ is the radial part of the S-state deuteron wave function. Our calculation in this Section follows the approach and notation of Ref. [8].

For the purposes of this exercise, we use the McGee wave function [11] for the deuteron. If another wave function (which fits the deuteron data) is used, the overlap integral changes only slightly. Since we are here only investigating the effect of the screening correction to the reaction rate, our specific choice of the deuteron wave function is unimportant.

The radial wave function $u_{pp}(r)$ satisfies the radial Schrodinger equation,

$$\frac{d^2u}{dr^2} - \left[\frac{1}{Rr} + V_{\text{nuc}}(r)\right]u = -k^2u, \tag{18}$$

where

$$R = \frac{\hbar^2}{2\mu e^2} = 28.8198 \text{ fm}, \tag{19}$$

$k = \mu v/\hbar$ is the center-of-mass momentum, and $V_{\text{nuc}}(r)$ is the short-range nuclear potential. For $V_{\text{nuc}}(r)$ we use an exponential potential which yields the observed value for the scattering length and effective range [8]. Again, the overlap integral turns out to be practically independent of the detailed shape of the nuclear potential (as long as it matches the measured scattering length and effective range), so the choice of nuclear potential is unimportant for determining the screening correction.

In the weak-screening case, Eq. (18) is replaced by

$$\frac{d^2u}{dr^2} - \left[\frac{e^{-r/r_D}}{Rr} + V_{\text{nuc}}(r)\right]u = -k^2u. \tag{20}$$

The solution to the Schrodinger equation is unique once the two boundary conditions are given. The first condition is $u(0) = 0$. The other boundary condition is obtained by noting that the asymptotic behavior of the wave function for $r \gg r_D$ must be [12],

$$u_{pp}^{\text{coul}}(r) \sim N_{\text{coul}} \sin\left(kr - \frac{1}{2kR}\log(2kr) + \delta_0^{\text{coul}}\right), \tag{21}$$

for the Coulomb potential, and

$$u_{pp}^{\text{sc}}(r) \sim N_{\text{sc}} \sin(kr - \delta_0^{\text{sc}}), \tag{22}$$

for the screened potential, where δ^{coul} and δ^{sc} are phase shifts. Fixing the incident flux of protons for the Coulomb and the screened-Coulomb interactions requires $N_{\text{coul}} = N_{\text{sc}}$.

To solve this boundary-value problem, we integrate Eqs. (18) and (20) from $r = 0$ with the condition $u(0) = 0$ and $u'(0) = 1$ to a large distance (about $10\,r_D$), and then test that the solutions converge to the form of Eqs. (21) and (22), respectively. From these numerical solutions, we obtain the normalizations N_{sc} and N_{coul}. We then use the calculated wave functions to evaluate the overlap integral in Eq. (17) both with and without screening. By squaring the ratio of the two overlap integrals, we determine numerically the screening correction to the cross section for the pp reaction.

In Fig. 1 we plot the WKB (dashed curve) and numerical (solid curve) results for the screening correction for the pp reaction as a function of relative momentum k. Our results show that the discrepancy is small. For values of k at which the pp reaction occurs ($k \simeq 0.016\,\text{fm}^{-1}$), the fractional difference is $O(10^{-4})$. In fact, at smaller k, the fractional difference is expected to be even smaller, as argued below. The increased discrepancy at smaller k shown in Fig. 1 is due to numerical error in our calculation: accurate integration of the Schrodinger equation becomes increasingly difficult at smaller k since the asymptotic forms in Eqs. (21) and (22) are reached at progressively larger r.
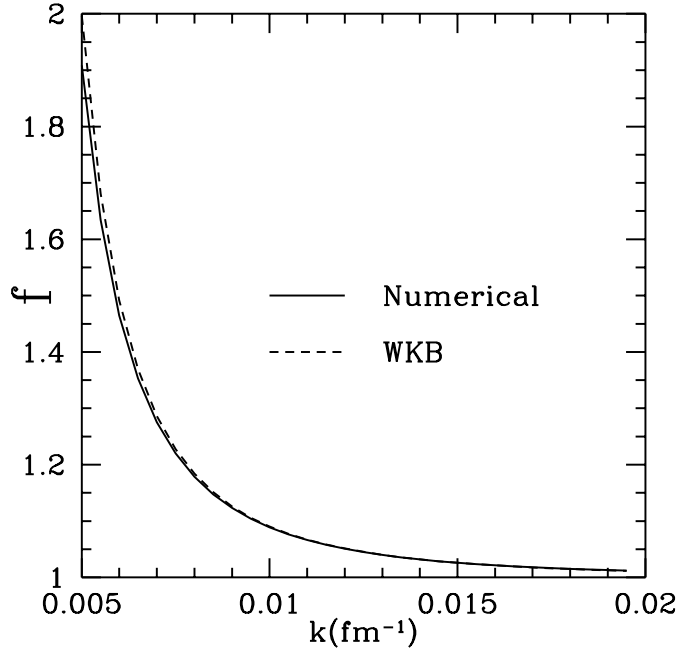
FIG. 1. The screening enhancement factor as a function of k. The dashed curve is that for the WKB result, and the solid curve is that for the numerical result.

IV. CONCLUSION

Our main result is that a numerical solution of the screened Schrodinger equation for the proton-proton reaction reaction gives results in excellent agreement [to $O(10^{-4})$] with the rate calculated analytically using the usual WKB approximation, as originally formulated by Salpeter.

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APPENDIX: A SMALL CORRECTION

In this Appendix, we calculate a correction to Salpeter's screening formula and find it to be negligibly small. The integral in Eq. (14) is usually evaluated by expanding in a power series of the inverse of a large quantity τ,

$$\tau = 3E_0/k_B T = 42.487(Z_1^2 Z_2^2 A T_6^{-1})^{1/3}. \tag{23}$$

The average product can then be written in a compact form [9]:

$$\langle \sigma v \rangle = 1.3005 \times 10^{-15} \left[\frac{Z_1 Z_2}{A T_6^2} \right]^{1/3} f_0 S_{\text{eff}} \exp(-\tau) \ \text{cm}^3\text{s}^{-1} \tag{24}$$

where S_{eff} is expressed in keV-barns. To first order in τ^{-1} [13],

$$S_{\text{eff}} = S(E_0) \left(1 + \tau^{-1} \left[\frac{5}{12} + \frac{5S'E_0}{2S} + \frac{S''E_0^2}{S} \right]_{E=E_0} \right). \tag{25}$$

Expressing the various quantities in terms of their values at $E = 0$, we find [13]

$$S_{\text{eff}}(E_0) \simeq S(0) \left[1 + \frac{5}{12\tau} + \frac{S'(E_0 + \frac{35}{36}k_B T)}{S} + \frac{S''E_0}{S} \left(\frac{E_0}{2} + \frac{89}{72}k_B T \right) \right]_{E=0}. \tag{26}$$

More accurately, however, we should include the factor $e^{x\pi\eta}$ in the thermal-average integral, Eq. (11). To do so, we rewrite the integral as

$$\langle \sigma v \rangle = \sqrt{\frac{8}{\pi\mu(k_B T)^3}} \int_0^\infty dE\, S(E) \exp(-2\pi\eta - E/k_B T + x\pi\eta). \tag{27}$$

Introducing the dimensionless quantity $z = E/E_0$, the exponential can be written as

$$-2\pi\eta - E/k_B T + x\pi\eta = -\frac{2\tau}{3}z^{-1/2} - \frac{\tau}{3}z + \frac{x_0\tau}{3}z^{-3/2}. \tag{28}$$

To first order in x_0, the minimum point of the exponent is thus shifted to $z = 1 - x_0$, or $E = E_0(1 - x_0)$. Using Laplace's method [14] for asymptotic expansion of integrals, we find that the only $O(x_0)$ correction to Eq. (24) is in the expression for S_{eff}. To order $O(\tau^{-1}, x_0)$, it is

$$S_{\text{eff}} = S(E) \left(1 + \tau^{-1} \left[\frac{5}{12} + \frac{5S'(E)E_0}{2S(E)} + \frac{S''(E)E_0^2}{S(E)} \right]_{E=E_0(1-x)} \right). \tag{29}$$

In other words, to first order in x_0, E_0 in Eq. (25) should be replaced by $E_0(1 - x_0)$. Expressed as $S(0)$, we have

$$S_{\text{eff}} \simeq S(0) \left[1 + \frac{5}{12\tau} + \frac{S'(0)(E_0(1-x) + \frac{35}{36}k_B T)}{S(0)} + \frac{S''(0)E_0}{S(0)} \left(\frac{E_0}{2}(1-2x) + \frac{89}{72}k_B T \right) \right], \tag{30}$$

where we have neglected terms of order $O(x_0/\tau)$. We see that there is an $O(x)$ correction to the S' and S'' terms. Since x is small ($\sim 10^{-2}$ for the pp reaction at the core of the Sun), and the S' and S'' terms are generally small compared with the lowest-order term, these corrections are very small, typically $\sim 0.1\%$. Therefore, the standard multiplicative correction factor (f_0) should give a screened interaction rate which is accurate to $O(1\%)$ in the weak-screening regime. Furthermore, since x_0 increases only very slowly with increasing mass number, the standard correction should also be accurate for other fusion reactions which are in the weak-screening regime.

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